

# WORKSHOP ON DYNAMIC X-RAY SCATTERING IN STRUCTURAL BIOLOGY

Advanced Photon Source, Argonne National Laboratory

November 2 – 4, 2011

## Program

### Crystallization Session

Wednesday Nov. 2 Afternoon

Bldg. 434 Conference Room C010	Crystallization devices designed for in situ diffraction at room temperature with and without flow cell capability will be demonstrated. Chair: Yu-sheng Chen, The University of Chicago
3:00 pm	Microfluidic platforms for protein crystallization Sarah Perry, University of California, Berkeley
3:30 pm	Crystallization devices for in situ diffraction at room temperature Zhong Ren, The University of Chicago
4:00 pm	Crystallization demo
5:00 pm	Sector 14 tours
Bldg. 400 Sector 14	Tour guides: Robert Henning and Vukica Srajer, The University of Chicago
6:00 – 8:00 pm Argonne Guest House	Dinner and reception

### Lecture Session I: Time-resolved crystallography

Thursday Nov. 3 Morning

Bldg. 402 Rm. E1100/1200	Experimental techniques in dynamic crystallography will be introduced and recent successful examples presented. This first Lecture Session focuses on time-resolved crystallography. Chair: Tim Graber, The University of Chicago
9:00 am	Coffee & rolls
9:50 am	Welcome Jim Viccaro, CARS Director, The University of Chicago
10:00 am	Overview of dynamic scattering studies at BioCARS Vukica Srajer, The University of Chicago
10:20 am	An introduction to the time-resolved facility at BioCARS Robert Henning, The University of Chicago
10:50 am	Five dimensional crystallography Marius Schmidt, University of Wisconsin, Milwaukee
11:30 am	Time-resolved experiments with monochromatic diffraction: large-angle rotation geometry (LARG) Zhong Ren, The University of Chicago
Noon, Bldg. 402 Gallery	Lunch
1:00 pm, Bldg. 401 front entrance stairs	Group photo Photographer: Guy Macha, The University of Chicago

### Lecture Session II: Time-resolved data analysis

Thursday Nov. 3 Afternoon

Bldg. 402 Rm. E1100/1200	A notable challenge of dynamic crystallography compared with static crystallography lies in data analysis and structural refinement. Participants will learn how to index, integrate and quantify Laue diffraction patterns. We will also demonstrate how a series of dynamic datasets can be analyzed jointly to illustrate time-dependent structural changes. Chair: Marius Schmidt, University of Wisconsin, Milwaukee
1:30 pm	Laue data collection and processing with Precognition™ Vukica Srajer, The University of Chicago
2:00 pm	Laue data analysis: creating feature-length electron density movies with TReX-II Friedrich Schotte, National Institutes of Health, NIDDK
2:30 pm	A global treatment of difference maps and simultaneous refinement of intermediate structures with dynamix Zhong Ren, The University of Chicago

Software Session Thursday Nov. 3 Afternoon – Evening		BioCARS Experiment Session Thursday Nov. 3 Afternoon – Evening	BioCAT Experiment Session Thursday Nov. 3 Afternoon
3:30 – 9:00 pm Bldg. 434 Conference Room C010 Chair: Vukica Srajer, The University of Chicago Computer software and test datasets will be set up for hands-on data processing. Datasets collected in the parallel Experiment Session may also be processed.		3:30 – 9:00 pm Bldg. 400 14-ID-B Chair: Robert Henning, The University of Chicago Attendees are invited to bring crystal samples to test Laue diffraction quality at room temperature. This is often the first step in developing time-resolved projects. We will demonstrate time-resolved data collection with photo-initiation by short laser pulses, and in situ diffraction procedures with novel crystallization devices.	3:30 – 6:00 pm Bldg. 400 18-ID Chair: Liang Guo, Illinois Institute of Technology BioCAT staff will demonstrate the stopped-flow capabilities of BioCAT beamline 18-ID for ms time scale kinetic solution scattering experiments.
7:00 pm, Bldg. 434 Conference Room C010	Pizza dinner provided		
Lecture Session III: Dynamic crystallography and scattering Friday Nov. 4 Morning			
Bldg. 402 Rm. E1100/1200	A real biological problem in structural dynamics often requires a unique technique that suits the specific project. Each topic in this second Lecture Session deviates slightly from standard pump-probe time-resolved crystallography and provides an example for widely applicable method for studies of structural dynamics. Time-resolved SAXS/WAXS and fiber diffraction, both of which are primary techniques of BioCAT and newly added capabilities of BioCARS, will also be discussed. Chair: Vukica Srajer, The University of Chicago		
8:30 am	Coffee & rolls		
9:00 am	Temperature scanning cryocrystallography: frozen dynamics Xiaojing Yang, The University of Chicago		
9:35 am	Meta-analysis: extracting dynamics from static structures Zhong Ren, The University of Chicago		
10:10 am	Coffee break		
10:30 am	Time-resolved SAXS/WAXS studies on the BioCARS beamline: probing protein structural dynamics in solution with 100-ps time resolution Philip Anfinrud, National Institutes of Health, NIDDK		
11:00 am	Capabilities for time-resolved SAXS on BioCAT beamline 18-ID Liang Guo, Illinois Institute of Technology		
11:30 am	Time-resolved fiber diffraction in a flow cell Irina Kosheleva, The University of Chicago		
Noon, Bldg. 402 Gallery	Lunch		
Case-study Session Friday Nov. 4 Afternoon			
1:30 – 4:00 pm Bldg. 434 Conference Room C010	We encourage attendees to present their specific systems in structural biology and prospects for dynamic X-ray scattering. This session provides an opportunity to identify promising experimental approaches, potential difficulties and feasible solutions. Participants are encouraged to participate in one-on-one discussions with BioCARS and BioCAT staff, and/or to present short talks or posters. Chair: Keith Moffat, The University of Chicago		